

BIRLA INSTITUTE OF TECHNOLOGY AND SCIENCE, PILANI

COMPREHENSIVE EXAMINATION (Closed Book)

I Semester 2016-17

DATE: 14-12-2016

Max Time: 60 min

Max Marks: 50

COMPUTATIONAL PHYSICS (PHY F313)

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1. Solution of Laplace equation: [3x10]

- (a) Suggest a numerical method to find out the solution of *Laplace* equation, $\nabla^2 V(\mathbf{r}) = 0$ in 2D.
- (b) How can you justify the basic assumptions of *Jacobi Relaxation* method that is sometimes used to find the potential at the required point.
- (c) Write down the psuedo code to execute the JR (or any other numerical method) method.

2. The charging of a capacitor in an *RC* circuit is represented by

$$R \frac{dq}{dt} = V - \frac{q}{C} \quad R = 100 \Omega, C = 150 \mu F, V = 12 V$$

with $q = 0, t = 0$. Use Euler method to solve (in 5 steps) and find out the $q(t = 0.005 \text{ s})$. Do you get the saturation in $q(t)$? Justify your answer. [20]

===== *—ALL THE BEST—*=====

BIRLA INSTITUTE OF TECHNOLOGY AND SCIENCE, PILANI
COMPREHENSIVE EXAMINATION (Open Source)

I Semester 2016-17

DATE: 14-12-2016

Max Marks: 70

COMPUTATIONAL PHYSICS (PHY F313)

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IMPORTANT

- You have to solve these problems by the codes you have written for your assignments.
 - The in-built functions of *MATLAB etc.* are **not allowed** to execute your codes.
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1. Solving the differential equations: [30]

(a) The two coupled I order equations

$$\frac{dy}{dt} = p \qquad \frac{dp}{dt} = -4\pi^2 y$$

represent SHM with period 1. Using your RK-4 codes, solve these equations with any particular initial conditions and investigate the accuracy with which system returns to its initial state at integral values of t .

(b) Solve the charging of capacitor problem (Q2 I part) by Improved Euler method. Plot the curve.

2. Consider a protein on a simple square lattice. The energy of model is defined as,

$$E = \sum_{\langle i,j \rangle} \delta_{ij} J_{A(i),A(j)}$$

where, the sum is over all pairs of proteins $\langle i, j \rangle$ in the chain and $\delta_{i,j} = 1$ if amino acids are nearest neighbour not connected by direct covalent bond. Consider 25 amino acids and assume that energy is measured in units of k_B and system is at temperature of 10. Using your Monte carlo codes (Metropolis based), simulate the different structures of protein. **[40]**

===== *—ALL THE BEST—* =====